10/552,595K Part with species Yong Chu 04/24/2009

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SESSION RESUMED IN FILE 'REGISTRY' AT 10:32:38 ON 24 APR 2009
FILE 'REGISTRY' ENTERED AT 10:32:38 ON 24 APR 2009
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COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   210.84   211.06

=> d his

     (FILE 'HOME' ENTERED AT 09:51:22 ON 24 APR 2009)

     FILE 'REGISTRY' ENTERED AT 09:51:38 ON 24 APR 2009
L1   STRUCTURE UPLOADED
L2   50 S L1
L3   STRUCTURE UPLOADED
L4   12498 S L1 FULL
                  SAVE L4 YC10552595/A
L5   STRUCTURE UPLOADED
L6   STRUCTURE UPLOADED
L7   STRUCTURE UPLOADED

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   211.32   211.54

FILE 'REGISTRY' ENTERED AT 10:33:00 ON 24 APR 2009
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STRUCTURE FILE UPDATES: 22 APR 2009 HIGHEST RN 1138219-76-7
DICTIONARY FILE UPDATES: 22 APR 2009 HIGHEST RN 1138219-76-7

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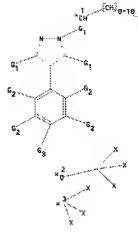
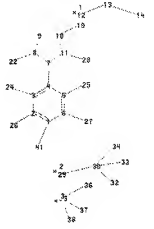
=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10552595\L14_04242009.str





chain nodes :
12 13 14 19 20 22 24 25 26 27 29 30 32 33 34 35 36 37 38 41
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
1-41 2-26 3-24 4-7 5-25 6-27 8-22 10-19 11-20 12-13 13-14 29-30 30-32
30-33 30-34 35-36 35-37 35-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
1-41 2-26 3-24 5-25 6-27 7-8 7-11 8-9 8-22 9-10 10-11 10-19 11-20 29-
30

exact bonds :
4-7 12-13 13-14 30-32 30-33 30-34 35-36 35-37 35-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:CH3,H,[*1]

G2:H,CH3

G3:G1,OH,SH,CN,NH2,NO2,X,[*2],[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 19:CLASS 20:CLASS 22:CLASS 24:CLASS
25:CLASS 26:CLASS
27:CLASS 29:CLASS 30:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS
41:CLASS

```
L8      STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l8 sam sss sub=l4
SAMPLE SUBSET SEARCH INITIATED 10:33:38 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -      639 TO ITERATE

100.0% PROCESSED      639 ITERATIONS                              3 ANSWERS
SEARCH TIME: 00.00.01

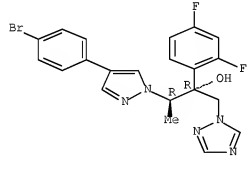
PROJECTIONS (WITHIN SPECIFIED SUBSET):          ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):       11264 TO    14296
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):              3 TO      163

L9            3 SEA SUB=L4 SSS SAM L8

=> d scan

L9   3 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-bromophenyl)-1H-pyrazol-
     1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)-
MF   C21 H18 Br F2 N5 O

Absolute stereochemistry.
```

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l8 full sss sub=l4
FULL SUBSET SEARCH INITIATED 10:34:21 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -     12498 TO ITERATE
```

100.0% PROCESSED 12498 ITERATIONS 59 ANSWERS
SEARCH TIME: 00.00.01

L10 59 SEA SUB=L4 SSS FUL L8

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 44.96 256.50

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FILE COVERS 1907 - 24 Apr 2009 VOL 150 ISS 18
FILE LAST UPDATED: 23 Apr 2009 (20090423/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

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=> s l10
L11 41 L10

=> save l11
ENTER NAME OR (END):yc10552595A/A
ANSWER SET L11 HAS BEEN SAVED AS 'YC10552595A/A'

=> d ibib abb hitstr 30-41
'ABB' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing

```
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

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FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

=> d ibib abs hitstr 30-41

L11  ANSWER 30 OF 41  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         1981:568095  CAPLUS  Full-text
DOCUMENT NUMBER:          95:168095
ORIGINAL REFERENCE NO.:   95:28085a,28088a
TITLE:                    Free-radical reactions of diazonium salts with
                          .alpha.,.beta.-unsaturated carbonyl compounds.  A new
                          synthesis of 1,4-diarylpyrazole derivatives
```

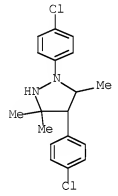
AUTHOR(S): Citterio, Attilio; Ramperti, Massimo; Vismara, Elena
CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy
SOURCE: Journal of Heterocyclic Chemistry (1981), 18(4), 763-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:168095

AB Free-radical decompn. of benzene diazonium salts catalyzed by titanous or titanous and ferrous salts in th presence of .beta.-substituted .alpha.,.beta.-unsatd. carbonyl compds., e.g., 4-methyl-3-pentene-2-one, Me 2-butenoate, leads to 1,4-diarylpyrazole derivs. The reaction occurs via an intermediate azo compds., which can be reduced by the metal salt or can be isolated and hydrogenated to pyrazole derivs.

IT 79481-66-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 79481-66-6 CAPLUS

CN Pyrazolidine, 1,4-bis(4-chlorophenyl)-3,3,5-trimethyl- (CA INDEX NAME)

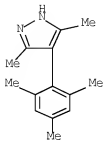


L11 ANSWER 31 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:179094 CAPLUS Full-text
DOCUMENT NUMBER: 84:179094
ORIGINAL REFERENCE NO.: 84:29023a,29026a
TITLE: Anisotropy effects of conjugated cyclic systems, I. NMR spectra of mesityl- and (9-anthryl)-substituted aromatic compounds
AUTHOR(S): Bock, Bodo; Kuhr, Manfred; Musso, Hans
CORPORATE SOURCE: Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1976), 109(3), 1184-94
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Magnetic anisotropies in mesityl and 9-anthryl derivs of benzene, mesitylene, anthracene, pyrimidine, pyrazole, and isoxazole were measured via 1H-NMR chem. shift data. The chem. shift differences of the 1-H and 4-H signals of 9-anthryl substituents are a measure of the magnetic anisotropy of arom. systems.

IT 55146-22-4
RL: PRP (Properties)
(NMR of)

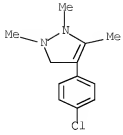
RN 59146-22-4 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(2,4,6-trimethylphenyl)- (CA INDEX NAME)



L11 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:175242 CAPLUS Full-text
DOCUMENT NUMBER: 82:175242
ORIGINAL REFERENCE NO.: 82:27995a,27998a
TITLE: Compositions of 1,2-dialkyl-3(and/or4)-aryl-3-pyrazolines and salts and method of lowering blood sugar levels with them
INVENTOR(S): Jacquier, Robert
PATENT ASSIGNEE(S): Schering A.-G., Fr.
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3818095	A	19740618	US 1972-243427	19720412

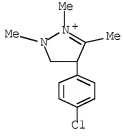
PRIORITY APPLN. INFO.: US 1972-243427 19720412
GI For diagram(s), see printed CA Issue.
AB 2-Pyrazolinium perchlorates (I) were prepd. and used in pharmaceutical compns. as hypoglycemics. Thus propiophenone [93-55-0], MeNHNHMe.2HCl [306-37-6], and HCHO [50-00-0] in EtOH with HCl were heated at reflux for 5 hr and worked up to give 1,2,4-trimethyl-3-phenyl-3-pyrazoline (II) [18508-29-7]. II (and other pyrazolines) were treated with HClO4 to give the perchlorate salts with a shift of the double bond to position 2. A tablet formulation contained, e.g., 50 mg/tablet 1,2,4-trimethyl-3-phenyl-2-pyrazolinium perchlorate [18075-75-7].
IT 51771-94-9P 51772-13-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51771-94-9 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl- (CA INDEX NAME)



RN 51772-13-5 CAPLUS
CN 1H-Pyrazolium, 4-(4-chlorophenyl)-4,5-dihydro-1,2,3-trimethyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 51772-12-4
CMF C12 H16 Cl N2



CM 2

CRN 14797-73-0
CMF Cl O4

L11 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:496468 CAPLUS Full-text
DOCUMENT NUMBER: 81:96468
ORIGINAL REFERENCE NO.: 81:15239a,15242a
TITLE: Compositions of 1,2-alkyl arylpyrazolium quaternary salts and lowering blood sugar levels with same

INVENTOR(S): Sherlock, Margaret
PATENT ASSIGNEE(S): Schering Corp.
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3818096	A	19740618	US 1972-243429	19720412

PRIORITY APPLN. INFO.: US 1972-243429 19720412

AB Compns. for lowering blood sugar levels in warm blooded animals suffering from hyperglycemia consist of a pharmaceutical carrier and I. Thus, to Ph3CCl in MeCN was added 1,2-dimethyl-3-phenyl-3-pyrazoline in MeCN to give after workupl,2-dimethyl-3-phenylpyrazolium chloride (II), m.p. 190-2.degree. (decompn.). Tablets are prepd. contg. II 100.00, confectioner's sugar (food grade) 123.00, polyvinylpyrrolidone (PVP) 10.00, corn starch (food grade, dried) 13.00, SiO2 2.00, and Mg sterate (U.S.P.) 2.00 mg/tablet. A damp mass consisting of II, the sugar, and PVP is prepd., dried, and reduced to granules. The starch, SiO2, and Mg stearate are added and mixed in. The compn. is then compressed into tablets.

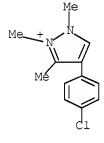
IT 54156-57-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(antihyperglycemic, prepn. of)

RN 54156-57-9 CAPLUS

CN 1H-Pyrazolium, 4-(4-chlorophenyl)-1,2,3-trimethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

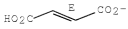
CRN 54156-56-8
CMF C12 H14 Cl N2



CM 2

CRN 18610-40-7
CMF C4 H3 O4

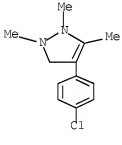
Double bond geometry as shown.



L11 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:120928 CAPLUS Full-text
DOCUMENT NUMBER: 80:120928
ORIGINAL REFERENCE NO.: 80:19467a,19470a
TITLE: Antiglycemic 3-pyrazolines
PATENT ASSIGNEE(S): Laboratoire Cetrane
SOURCE: Fr. Demande, 39 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2179559	A1	19731123	FR 1972-12761	19720412
FR 2179559	B1	19750425		
PRIORITY APPLN. INFO.:			FR 1972-12761	19720412

GI For diagram(s), see printed CA Issue.
AB Pyrazoles I, II, and III (R = Me, Ph, substituted phenyl; R1 = H, Me, Et, Ph, p-ClC6H4; R2 = H, Me, Ph; X = ClO4, iodide, fumarate) (56 compds.), were prepd. Condensation of RCOCHR1CH2R2 or RCOCHR1COR2 with MeNHNHMe.2HCl and paraformaldehyde gave I or II, resp. LiAlH4 redn. of II gave pyrazolinium III.
IT 51771-94-9P 51772-13-5P 51772-18-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51771-94-9 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl- (CA INDEX NAME)

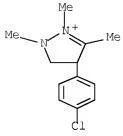


RN 51772-13-5 CAPLUS
CN 1H-Pyrazolium, 4-(4-chlorophenyl)-4,5-dihydro-1,2,3-trimethyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 51772-12-4

CMF C12 H16 Cl N2



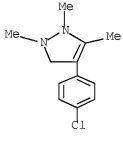
CM 2

CRN 14797-73-0
CMF Cl O4

RN 51772-18-0 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl-,
(2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 51771-94-9
CMF C12 H15 Cl N2

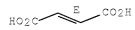


CM 2

CRN 110-17-8

CMF C4 H4 O4

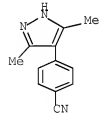
Double bond geometry as shown.



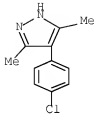
L11 ANSWER 35 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:108434 CAPLUS Full-text
DOCUMENT NUMBER: 80:108434
ORIGINAL REFERENCE NO.: 80:17443a,17446a
TITLE: Reactivity of 4-diazo-3,5-dimethylpyrazole. IV. Catalytic action of hydroquinone in the Gomberg-Bachmann reaction
AUTHOR(S): Fukata, Gouki; Kawazoe, Yuichi; Taguchi, Tanezo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, Japan
SOURCE: Yakugaku Zasshi (1974), 94(1), 36-43
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Refluxing 4-diazo-3,5-dimethylpyrazole (I) in benzene for a long time afforded 4-phenyl-3,5-dimethylpyrazole, 1H,4H-3-methylpyrazolo[4,3-c]-pyrazole, 3,5-dimethylpyrazole, and biphenyl in 36, 15, 12, and 7% yields, resp. Replacement of benzene with nitrobenzene in this reaction gave o-, m-, and p-isomers of 4-(nitrophenyl)-3,5-dimethylpyrazole in a ratio of 10:2.8:3.0. In these reactions, addn. of hydroquinone (catalytic quantity, 5% by wt. of I) was very effective in increasing the yield of 4-aryl-3,5-dimethylpyrazole and reduction of reaction time. The intermediate in these reactions was a diazonium salt which was formed by the addn. of one mole of hydroquinone to two moles of I.

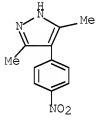
IT 51463-73-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in benzonitrile)
RN 51463-73-1 CAPLUS
CN Benzonitrile, 4-(3,5-dimethyl-1H-pyrazol-4-yl)- (CA INDEX NAME)



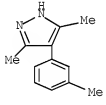
IT 51463-76-4P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in chlorobenzene)
RN 51463-76-4 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-3,5-dimethyl- (CA INDEX NAME)



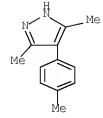
IT 42418-61-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in nitrobenzene)
RN 42418-61-1 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(4-nitrophenyl)- (CA INDEX NAME)



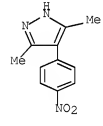
IT 51463-81-1P 51463-82-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in toluene)
RN 51463-81-1 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(3-methylphenyl)- (CA INDEX NAME)



RN 51463-82-2 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(4-methylphenyl)- (CA INDEX NAME)

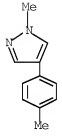


L11 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:452480 CAPLUS Full-text
DOCUMENT NUMBER: 79:52480
ORIGINAL REFERENCE NO.: 79:8467a,8470a
TITLE: Reactivity of 4-diazo-3,5-dimethylpyrazole
AUTHOR(S): Fukata, Gouki; Kawazoe, Yuichi; Taguchi, Tanezo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, Japan
SOURCE: Tetrahedron Letters (1973), (15), 1199-200
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compd. (I) was heated in Me3COH-AcOH, Me3COH, and EtOH to give 70% II, 45% III, and 85% MeCHO resp. Heating I in C6H6 gave 15% II, 12% 3,5-dimethylpyrazole, 7% biphenyl, and 36% IV. Hydroquinone and benzoquinone catalyzed the reaction giving IV (68%). III was also obtained by coupling I with II in Me3COH. Heating I in PhNO2 gave 4-nitrophenyl-3,5-dimethylpyrazole with a ratio of o:m:p-isomers = 10:3:3.
IT 42418-61-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 42418-61-1 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(4-nitrophenyl)- (CA INDEX NAME)

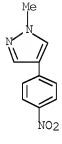


L11 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:539882 CAPLUS Full-text
DOCUMENT NUMBER: 77:139882
ORIGINAL REFERENCE NO.: 77:23001a,23004a
TITLE: Pyrazoles. IX. Nitration of 1-methyl-4-phenylpyrazole
AUTHOR(S): Cohen-Fernandes, Pauline; Habraken, Clarisse L.
CORPORATE SOURCE: Gorlaeus Lab., Univ. Leiden, Leiden, Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1972), 91(9-10), 1185-92
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The phenyl and the pyrazole ring were both substituted on nitration with acetyl nitrate and a predominant ortho substitution in the phenyl ring was obsd. The pyrazole ring was susceptible to nitration at positions other than the, hitherto favored, 4-position.
IT 37921-11-2P 37921-15-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 37921-11-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



RN 37921-15-6 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-nitrophenyl)- (CA INDEX NAME)



L11 ANSWER 38 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:46687 CAPLUS Full-text
DOCUMENT NUMBER: 58:46687
ORIGINAL REFERENCE NO.: 58:7921a-c
TITLE: Derivatives of 3-substituted pyrazolones and 3-substituted pyrazolines
AUTHOR(S): Kurihara, Tozaburo; Takeda, Hideo; Iino, Naoko
CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai
SOURCE: Tohoku Yakka Daigaku Kiyo (1961), 8, 103-9
CODEN: TYDKAG; ISSN: 0372-347X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB 1-Phenyl-3-chloro-4-pyrazoolone (1.9 g.) was warmed with 0.9 g. Me2NH in MeOH in an autoclave 2 hrs. to give 1-phenyl-3-dimethylamino-5-pyrazolone, m. 132.degree. (EtOH). Similarly prepd. were the following I (R, R1, R2, and m.p. given): H, H, NEt2, 131.degree.; H, H, (iso-Bu)2 N, 108.degree.; H, Br, (iso-Bu)2 N, 138-40.degree.; H, Cl, (iso-Bu)2N, 126.degree.; H, H, piperidyl, 139.degree.; H,H, morpholyl, 134.degree.; Bu, H, morpholyl, 225.degree.; H, Br, morpholyl, 165.degree.; H, Cl, morpholyl, 143.degree.; H. Me, morpholyl, 168-170.degree.; H, OMe, morpholyl, 127-30.degree.; H, H, Et2NCH2NH, 202.degree.; H, H, Et2NCH2CONH, 158.degree.; H, H, morpholylacetamido.

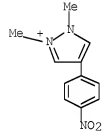
IT 94628-08-7
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 94628-08-7 CAPLUS

CN 1H-Pyrazolium, 1,2-dimethyl-4-(4-nitrophenyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 94628-07-6
CMF C11 H12 N3 O2



CM 2

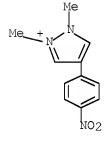
CRN 14797-73-0
CMF Cl O4

L11 ANSWER 39 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:46686 CAPLUS Full-text
DOCUMENT NUMBER: 58:46686
ORIGINAL REFERENCE NO.: 58:7920h,7921a
TITLE: The 1,2-dithiolium cation. A new pseudoaromatic system. III. Conversion of dithiolium salts to quaternary pyrazolium salts and dithiolethiones
AUTHOR(S): Klingsberg, Erwin

CORPORATE SOURCE: Am. Cyanamid Co., Bound Brook, NJ
SOURCE: Journal of Organic Chemistry (1963), 28, 529-30
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:46686
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 16791e. 4-Phenyl-(I) and 4-p-nitrophenyl-1,2-dithiolium salts react with N,N'-disubstituted hydrazines to give N,N-disubstituted pyrazolium salts, e.g., II, and with sulfur to give 1,2-dithiole-3-thiones, e.g. III.
IT 94628-08-7P, 1,2-Dimethyl-4-(p-nitrophenyl)pyrazolium perchlorate
RL: PREP (Preparation)
(prepn. of)
RN 94628-08-7 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-4-(4-nitrophenyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 94628-07-6
CMF C11 H12 N3 O2



CM 2

CRN 14797-73-0
CMF Cl O4

L11 ANSWER 40 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:55872 CAPLUS Full-text
DOCUMENT NUMBER: 52:55872
ORIGINAL REFERENCE NO.: 52:10061i,10062a-c
TITLE: Synthesis of 2-substituted-acenaphtheno(4',5'-4,5)imidazole derivatives
AUTHOR(S): Saikachi, Haruo; Tsuge, Otohiko; Yoshimura, Kazuki

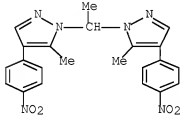
CORPORATE SOURCE: Kyushu Univ., Fukuoka
SOURCE: Kogyo Kagaku Zasshi (1956), 59, 933-6
CODEN: KGKZA7; ISSN: 0368-5462
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 52, 3779e. 4-Nitro-5-acylaminoacenaphthenes (I) (formyl, m. 226-7.degree.; Ac, 241.5-2.0.degree.; Bz, 228-9.degree.) were obtained from 5-amino-acenaphthene through the 5-acylaminoacenaphthene. Formyl and Ac derivs. of I were hydrolyzed by heating with EtOH-HCl 20 hrs. to give 4-nitro-5-aminoacenaphthene (II), m. 212-13.degree.. II was reduced with SnCl in HCl satd. EtOH to give 4,5-diaminoacenaphthene (III), m. 137.degree.. III (1 g.) with 3 cc. boiling 80% HCO2H gave 0.6 g. acenaphtheno(4',5'-4,5)imidazole, m. 221-2.degree.. III (1 g.) with 2 cc. Ac2O in C6H6 on an H2O bath gave 0.6 g. 1-(N-acetyl)-2-methyl-acenaphtheno(4',5'-4,5)imidazole (IV), m. 263.degree.. Ac deriv. of I was reduced in Ac2O by Zn and converted to IV. The reduction of formyl deriv. of I in Ac2O with Zn by boiling gave 1-(N-carboxy) - 2 - methylacenaphtheno(4',5' - 4,5)imidazole, m. 279.degree., sol. in aq. NaOH. 4,5-Dibenzoyldiaminoacenaphthene, m. 282-3.degree., was obtained by boiling III with BzCl. III.HCl (1 g.) heated with 0.3 g. urea at 150-5.degree. 45 min. and extd. with aq. NaOH and then EtOAc gave acenaphtheno-(4',5'-4,5)-2-imidazolinone, m. above 340.degree.. Similarly, III.HCl with thiourea at 230.degree. or 450.degree. gave acenaphtheno-(4',5'-4,5)-2-thioimidazolinone, m. above 340.degree..

IT 102599-03-1P, Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)-
RL: PREP (Preparation)
(prepn. of)

RN 102599-03-1 CAPLUS

CN Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)- (6CI) (CA INDEX NAME)



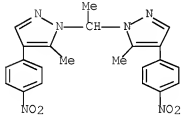
L11 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:55871 CAPLUS Full-text
DOCUMENT NUMBER: 52:55871
ORIGINAL REFERENCE NO.: 52:10061e-i
TITLE: Products from the reaction of diazoethane with diazoketones
AUTHOR(S): Yates, P.; Farnum, D. G.; Wiley, D. W.
CORPORATE SOURCE: Harvard Univ.
SOURCE: Chemistry & Industry (London, United Kingdom) (1958) 69-70
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 43, 4652g, 6992e. The structures ArCOCR:NN:CHR' (R = R' = Me) (I) and (R = H, R' = Me) (II) (Ar = p-O2NC6H4 throughout) previously proposed (C.A. 43, 6992e) for the products of the reaction between ARCOCRN2 and MeCHN2 were confirmed. I, m. 99-100.degree., .lambda. 265 m.mu. (.epsilon. 13,700), .lambda. 5.93, 6.06, 6.23 .mu., boiled 15 min. with 70% EtOH gave (ArCOCMe:NNH)2CHMe (III), m. 159-60.degree., .lambda. 268 and 315 m.mu. (.epsilon. 35,300 and 18,900), .lambda. 3.04, 6.03 (shoulder), 6.06, 6.24, 6.39 .mu., corresponding to the earlier compd., C11H9O2N3 (C.A. 43, 6992e). III with Ac2O and NaOAc gave ArCOCMe:NNHAc, m. 165.5-6.5.degree., .lambda. 245 and 278 m.mu. (.epsilon. 12,100 and 19,300), .lambda. 3.04, 5.81, 5.92, 5.99, 6.26 .mu., identical with the acetylated product of ArCOCMe:NNH2 (IV), m. 173-3.2.degree., .lambda. 274 m.mu. (.epsilon. 14,200), .lambda. 2.92, 3.03, 3.31, 6.04, 6.16, 6.25, 6.36 .mu., obtained by NH4HS reduction of ArCOCMeN2. III with BzH gave ArCOCMe:NN:CHPh, m. 114.5-15.5.degree., .lambda. 5.98, 6.18, 6.23, 6.40 .mu., also obtained from IV. I with IV 6 days in CHCl3 or refluxing in abs. EtOH gave III (63% yield by the 2nd method). I heated alone in abs. EtOH gave ArCOCMe:NNHCHMeOEt, m. 126-7.degree., .lambda. 268 and 305 m.mu. (.epsilon. 17,750 and 11,000), .lambda. 3.03, 6.08, 6.24, 6.42 .mu., which was converted to III by treatment with aq. EtOH. ArCOCHN2 with MeCHN2 gave the 2 stereoisomers of II, A, m. 69-70.degree., .lambda. 5.93, 6.09, 6.22 .mu., B, m. 121-2.degree. (decompn.), .lambda. 5.99, 6.09, 6.24, 6.29 .mu.; A was converted to B by heating at its m.p. Further reaction of II with MeCHN2 gave ArCOCMe:CHNHN:CHMe (V), m. 136-6.5..degree., .lambda. 298 m.mu. (.epsilon. 22,800), .lambda. 3.02, 6.08, 6.16, 6.31 .mu., corresponding to the earlier compd. (C.A. 43, 6992e), C14H17O3N3. Hydrolysis of V in cold 2N HCl gave 3-(p-nitrophenyl)-4-methylpyrazole (VI), m. 181.5-2.degree., .lambda. 2.92, 3.13, 6.23 .mu., identified by nitration of the Ph analog, and [ArC:CMe.CH:N.N]2CHMe, m. 201.5-2.5.degree., .lambda. 231 and 318 m.mu. (.epsilon. 22,500 and 21,800), .lambda. 6.24 and 6.44 .mu.. Ultraviolet spectra were taken in CH2Cl2, infrared spectra in CHCl3.

IT 102599-03-1P, Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)-
RL: PREP (Preparation)
(prepn. of)

RN 102599-03-1 CAPLUS

CN Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)- (6CI) (CA INDEX NAME)



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PASSWORD:
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | 0.00 | -9.84

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L3 STRUCTURE UPLOADED
L4 12498 S L1 FULL
SAVE L4 YC10552595/A
L5 STRUCTURE UPLOADED
L6 STRUCTURE UPLOADED
L7 STRUCTURE UPLOADED

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FILE 'CAPLUS' ENTERED AT 10:44:41 ON 24 APR 2009
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ring nodes :
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exact bonds :
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normalized bonds :
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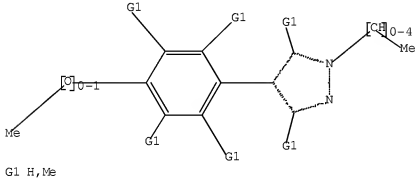

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FILE LAST UPDATED: 23 Apr 2009  (20090423/ED)

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substance identification.

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L16 15 L15

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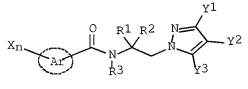
L16 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:636634 CAPLUS Full-text
DOCUMENT NUMBER: 149:10000
TITLE: Preparation of novel pyrazole derivatives as harmful organism control agents, and use of the control agents
INVENTOR(S): Tanaka, Koji; Hasebe, Motohiro; Kuroki, Nobutaka; Suwa, Akiyuki
PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 138pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008062878	A1	20080529	WO 2007-JP72682	20071122

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: JP 2006-316296 A 20061122
OTHER SOURCE(S): MARPAT 149:10000
GI



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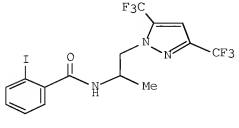


II

AB N-2-(substituted pyrazolyl)ethylcarboxamide derivs. represented by the general formula (I) or salts thereof [R1, R2 = H, C1-6 alkyl; or R1 and R2 together form C3-6 cycloalkane; R3 = H, C1-6 alkyl, C1-6 alkoxy-C1-6 alkyl, C1-6 alkylcarbonyl, C1-6 alkoxycarbonyl; Ar = Ph, pyridyl, pyrimidinyl, pyrazinyl, pyrazolyl, furyl, thienyl, oxazolyl, isoxazolyl, thiazolyl, isothiazolyl, thiadiazolyl; X = halo, cyano, NO2, C1-6 alkyl, halo-C1-6 alkyl, C3-6 cycloalkyl, C1-6 alkoxy, halo-C1-6 alkoxy, C1-6 alkylthio, halo-C1-6 alkylthio, C1-6 alkoxy-C1-6 alkylthio, C1-6 alkylsulfinyl, halo-C1-6 alkylsulfinyl, C1-6 alkylsulfonyl, halo-C1-6 alkylsulfonyl, NH2, mono- or di(C1-6 alkyl)amino, each ring-(un)substituted piperidino, Ph, PhO, phenyl-C1-6 alkyl, C1-6 alkoxyimino-C1-6 alkyl; n = an integer of 0-5; Y1, Y2, Y3 = H, halo, cyano, C1-6 alkyl, halo-C1-6 alkyl, C1-6 alkylcarbonyl, C1-6 alkoxy, halo-C1-6 alkoxy, C1-6 alkoxy-C1-6 alkyl, C1-6 alkylthio, halo-C1-6 alkylthio, C1-6 alkylsulfinyl, halo-C1-6 alkylsulfinyl, C1-6 alkylsulfonyl, halo-C1-6 alkylsulfonyl, NH2, mono- or di(C1-6 alkyl)amino, CONH2, mono- or di(C1-6 alkyl)carbamoyl, each (un)substituted Ph, heterocyclyl, or heterocyclylcarbonyl, etc.; or adjacent two Xs, Y1 and Y2, or Y2 and Y3 represent C3-5 alkylene, C3-5 alkenylene, C1-3 alkylenedioxy, or halo-C1-3 alkylenedioxy] were prepd. There is also disclosed a harmful organism control agent comprising the deriv. or the salt thereof as an active ingredient. These compds. exhibit controlling effect on plant pests with a wide spectrum of fungicidal or nematocidal activity. Thus, 0.26 g 2-[3,5-bis(trifluoromethyl)pyrazol-1-yl]-1- methylethylamine was mixed with 10 mL THF, followed by adding sequentially Et3N 0.30, 2-iodobenzoic acid 0.25, and 2-chloro-1-methylpyridinium iodide 0.31 g, and the resulting mixt. was stirred for 2 h to give 79% N-[2-[3,5-bis(trifluoromethyl)pyrazol-1-yl]-1-methylethyl]-2-iodobenzamide (II). II at 200 ppm controlled .gtoreq.70-79% Alternaria brassicae on cabbage leaves and Blumeria graminis hordei on barley seedlings.

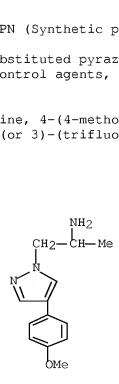
IT 1029414-87-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of N-2-(substituted pyrazolyl)ethylcarboxamide derivs. as harmful organism control agents, in particular fungicides and nematocides)

RN 1029414-87-6 CAPLUS

CN 1H-Pyrazole-1-ethanamine, 4-(4-methoxyphenyl)-.alpha.,3(or .alpha.,5)-dimethyl-5(or 3)-(trifluoromethyl)-, (.alpha.S)- (CA INDEX NAME)



D1—Me

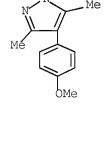
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:614394 CAPLUS Full-text
DOCUMENT NUMBER: 147:234920
TITLE: New Catalysts for Suzuki-Miyaura Coupling Reactions of Heteroatom-Substituted Heteroaryl Chlorides
AUTHOR(S): Guram, Anil S.; Wang, Xiang; Bunel, Emilio E.; Faul, Margaret M.; Larsen, Robert D.; Martinelli, Michael J.
CORPORATE SOURCE: Chemistry Research and Discovery, Amgen Inc., Thousand Oaks, CA, 91320-1799, USA
SOURCE: Journal of Organic Chemistry (2007), 72(14), 5104-5112 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:234920

AB The new air-stable PdCl2{PR2(Ph-R')}2 complexes, readily prepd. from com. reagents, exhibit unique efficiency as catalysts for the Suzuki-Miyaura coupling reactions of a variety of heteroatom-substituted heteroaryl chlorides with a diverse range of aryl/heteroaryl boronic acids. The coupling reactions catalyzed by the new complexes exhibit high product yields (88-99%) and high catalyst turnover nos. (up to 10,000 TON).

IT 887919-41-7P, 4-(4-Methoxyphenyl)-1,3,5-trimethyl-1H-pyrazole
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalytic Suzuki-Miyaura coupling reactions of heteroatom-substituted heteroaryl chlorides with aryl/heteroaryl boronic acids)

RN 887919-41-7 CAPLUS
CN 1H-Pyrazole, 4-(4-methoxyphenyl)-1,3,5-trimethyl- (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:509883 CAPLUS Full-text
DOCUMENT NUMBER: 146:501057
TITLE: Antifungal triazole derivatives, processes for preparing them, and pharmaceutical compositions containing them
INVENTOR(S): Park, Joon Seok; Yu, Kyung A.; Kim, Sun Young; Song, Yeon Jung; Kim, Kang-Pil; Yoon, Yun Soo; Han, Mi Ryeong
PATENT ASSIGNEE(S): Daewoong Pharmaceutical Co., Ltd., S. Korea
SOURCE: PCT Int. Appl., 62pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007052943	A1	20070510	WO 2006-KR4495	20061031
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1951705	A1	20080806	EP 2006-812334	20061031
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2009513698	T	20090402	JP 2008-538814	20061031
US 20080287440	A1	20081120	US 2008-92156	20080430
IN 2008DN04370	A	20080815	IN 2008-DN4370	20080522
KR 2008088583	A	20081002	KR 2008-712856	20080528
CN 101365692	A	20090211	CN 2006-80049309	20080626

PRIORITY APPLN. INFO.: KR 2005-103142 A 20051031
WO 2006-KR4495 W 20061031

GI

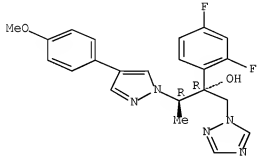
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to antifungal triazole derivs. I, processes for prepg. them, and pharmaceutical prepns. comprising them. In compd. I, Ar is C6-20 aryl substituted with .gtoreq. 1 halo or CF3; R1 is H, F, or C1-4 alkyl; R2, R3, and R4 independently represent H, halo, NO2, CN, NH2, OH, (cyclo|halo)alkyl, alkoxy, (un)substituted (hetero)aryl; including pharmaceutically acceptable salts thereof. For instance, the invention compd. II was prepd. by protection of 4-bromo-1H-pyrazole with trityl chloride followed by cross-coupling with 4-fluorophenylboronic acid (51%), deprotection (81%), and addn. to compd. III (56%). The antifungal activities of I were tested, e.g., the invention compd. IV had MIC values of .ltoreq. 0.015 .mu.g/mL against Candida albicans, 0.25 .mu.g/mL against Candida krusei, etc.

IT 936357-31-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn. of antifungal triazole derivs.)
RN 936357-31-2 CAPLUS
CN 1H-1,2,4-Triazole-1-ethanol, .alpha.-(2,4-difluorophenyl)-.alpha.-[(1R)-1-[4-(4-methoxyphenyl)-1H-pyrazol-1-yl]ethyl]-, (.alpha.R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:218467 CAPLUS Full-text
DOCUMENT NUMBER: 146:274490
TITLE: Transition metal complexes of N-heterocyclic carbenes, method of preparation and use in transition metal catalyzed organic transformations
INVENTOR(S): O'Brien, Christopher J.; Organ, Michael G.; Kantchev, Assam B.
PATENT ASSIGNEE(S): Total Synthesis Ltd., Can.
SOURCE: Can. Pat. Appl., 65pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CA 2556850	A1	20070224	CA 2006-2556850		20060823
CA 2551412	A1	20070224	CA 2006-2551412		20060630
US 20070073055	A1	20070329	US 2006-508334		20060823
US 7250510	B2	20070731			
PRIORITY APPLN. INFO.:			US 2005-710487P	P	20050824
			US 2005-710869P	P	20050825
			CA 2006-2551412	A	20060630
			US 2006-817343P	P	20060630

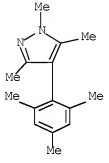
OTHER SOURCE(S): CASREACT 146:274490; MARPAT 146:274490
AB The present invention relates to catalysts of transition metal complexes of N-heterocyclic carbenes, their methods of prepn. and their use in chem. synthesis. The synthesis, ease-of-use, and activity of the compds. of the present invention are substantial improvements over in situ catalyst generation. Further, the transition metal complexes of N-heterocyclic

carbenes of the present invention may be used as pre-catalysts in metal-catalyzed cross-coupling reactions.

IT 927706-68-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use of palladium N-heterocyclic carbenes in catalyzed org. transformations)

RN 927706-68-1 CAPLUS

CN 1H-Pyrazole, 1,3,5-trimethyl-4-(2,4,6-trimethylphenyl)- (CA INDEX NAME)



L16 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:23439 CAPLUS Full-text

DOCUMENT NUMBER: 146:295309

TITLE: Biaryls made easy: PEPPSI and the Kumada-Tamao-Corriu reaction

AUTHOR(S): Organ, Michael G.; Abdel-Hadi, Mirvat; Avola, Stephanie; Hadei, Niloufar; Nasielski, Joanna; O'Brien, Christopher J.; Valente, Cory

CORPORATE SOURCE: Dep. Chem., York Univ., Toronto, ON, M3J 1P3, Can.

SOURCE: Chemistry--A European Journal (2006), 13(1), 150-157
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:295309

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB An easily employed, highly versatile Kumada-Tamao-Corriu (KTC) protocol utilizing the PEPPSI (Pyridine, Enhanced, Precatalyst, Prepn., Stabilization and Initiation) precatalysts I and II is detailed. The ease-of-use of these catalysts and the synthesis of a wide range of hindered biaryls, large coupling partners, and drug-like heterocycles, in high yield, makes the PEPPSI-KTC protocol very attractive. E.g., I catalyzed the cross-coupling of 4-ClC6H4OMe and 4-MeC6H4MgBr to give 85% biaryl III. The high reactivity of the PEPPSI system allowed a tetra-ortho-substituted heterocycle IV to be synthesized at room temp. for the first time using any protocol. The PEPPSI protocols also tolerated the Boc protecting group and phenols required no protection in modified conditions. A relatively large scale (10 g) reaction was also performed with no loss in performance. Furthermore, I was compared

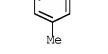
to previously reported highly active phosphine ligands, e.g. tricyclopropylphosphine, and was shown to result in significantly better yields under identical conditions. Finally, the authors demonstrated that the PEPPSI catalyst system is very adept at performing sequential KTC coupling reactions, analogous to multicomponent reactions, which allow complex polyaryl and polyheteroaryl architectures to be produced in one single operation.

IT 927706-68-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of biaryls via Kumada-Tamao-Corriu cross-coupling reaction of aryl halides or alcs. with Grignard reagents utilizing PEPPSI precatalysts)

RN 927706-68-1 CAPLUS

CN 1H-Pyrazole, 1,3,5-trimethyl-4-(2,4,6-trimethylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:302956 CAPLUS Full-text

DOCUMENT NUMBER: 145:8119

TITLE: New air-stable catalysts for general and efficient Suzuki-Miyaura cross-coupling reactions of heteroaryl chlorides

AUTHOR(S): Guram, Anil S.; King, Anthony O.; Allen, John G.; Wang, Xianghong; Schenkel, Laurie B.; Chan, Johann; Bunel, Emilio E.; Faul, Margaret M.; Larsen, Robert D.; Martinelli, Michael J.; Reider, Paul J.

CORPORATE SOURCE: Chemistry Research and Discovery, Amgen Inc., Thousand Oaks, CA, 91320, USA

SOURCE: Organic Letters (2006), 8(9), 1787-1789
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:8119

AB Air-stable PdCl2{PtBu2(p-R-Ph)}2 (R = H, NMe2, CF3,) complexes represent simple, general, and efficient catalysts for the Suzuki-Miyaura cross-coupling reactions of aryl halides including five-membered heteroaryl halides and heteroatom-substituted six-membered heteroaryl chlorides with a diverse range of arylboronic acids. High product yields and turn-over-nos. (10 000 TON) were obsd.

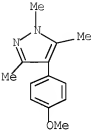
IT 887919-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of biaryls via palladium-catalyzed Suzuki-Miyaura

cross-coupling reaction of aryl or heteroaryl chlorides or bromotrimethylpyrazole with arylboronic acids)

RN 887919-41-7 CAPLUS

CN 1H-Pyrazole, 4-(4-methoxyphenyl)-1,3,5-trimethyl- (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:872790 CAPLUS Full-text

DOCUMENT NUMBER: 141:350155

TITLE: Preparation of phenyl-substituted heterocycles as MIF inhibitors for the treatment of inflammatory diseases

INVENTOR(S): Morand, Eric Francis; Iskander, Magdy Naguib; Skene, Colin Edward

PATENT ASSIGNEE(S): Cortical Pty. Ltd., Australia

SOURCE: PCT Int. Appl., 144 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089927	A1	20041021	WO 2004-AU453	20040407
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004228069	A1	20041021	AU 2004-228069	20040407
CA 2521606	A1	20041021	CA 2004-2521606	20040407
EP 1611120	A1	20060104	EP 2004-726068	20040407
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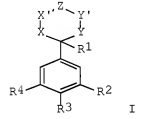
JP 2006522025	T	20060928	JP 2006-504000	20040407
US 20070010563	A1	20070111	US 2005-552595	20051007
IN 2005KN02068	A	20060922	IN 2005-KN2068	20051021

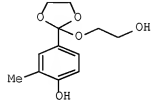
ZA 2005008847	A	20061025	ZA 2005-8847		20051101
IN 2008KN02178	A	20090116	IN 2008-KN2178		20080530
PRIORITY APPLN. INFO.:			AU 2003-901579	A	20030407
			AU 2003-906773	A	20031208
			WO 2004-AU453	W	20040407
			IN 2005-KN2068	A3	20051021

OTHER SOURCE(S): MARPAT 141:350155

GI



I



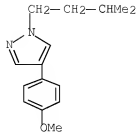
II

AB Title compds. I [wherein X, X', Y, Y' = independently C(R5)2, O, S, NR5; Z = a bond, C(R5)2, O, S, NR5; or XX', YY', X'Z, or Y'Z = CR5=CR5, CR5=N, N=CR5, N=N; R1 = H, alkyl, alkenyl, alkynyl, acyl, alkoxy, alkylthio, amino, etc.; R2, R4 = independently H, alkyl, hydroxy(alkyl), mercapto(alkyl), haloalkyl, nitroalkyl, etc.; R3 = alkyl, hydroxy(alkyl), mercapto(alkyl), haloalkyl, nitroalkyl, (hetero)aryl(alkyl), etc.; with provisos; or pharmaceutically acceptable salts or prodrugs thereof] were prepd. for inhibiting the cytokine or biol. activity of macrophage migration inhibitory factor (MIF). Examples include syntheses for forty-five invention compds. and eight bioassays. For instance, reaction of 3-methyl-4-hydroxybenzaldehyde with ethylene glycol in the presence of p-toluenesulfonic acid in toluene provided the dioxolane II (24%). The latter significantly inhibited the induction of S112 human fibroblast proliferation at 1 nM and suppressed MIF-dependent IL-1 induced fibroblast cyclooxygenase-2 expression by 10.5% at 0.01 .mu.M up to 31.4% at 50 .mu.M. No cytotoxicity, i.e., no significant increase in apoptotic cells or decrease in viable cells, resulted from treatment of S112 human dermal fibroblasts with therapeutic concns. (50 .mu.M) of II. Thus, I and their pharmaceutical compns. are useful for treating autoimmune diseases, tumors, or inflammatory diseases.

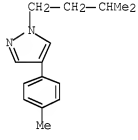
IT 777063-40-8P, 4-(4-Methoxyphenyl)-1-(3-methylbutyl)-1H-pyrazole
777063-42-0P, 1-(3-Methylbutyl)-4-(4-methylphenyl)-1H-pyrazole
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(MIF inhibitor; prepn. of Ph-substituted heterocycles as MIF inhibitors for treatment of inflammatory diseases, tumors, or autoimmune diseases)

RN 777063-40-8 CAPLUS

CN 1H-Pyrazole, 4-(4-methoxyphenyl)-1-(3-methylbutyl)- (CA INDEX NAME)



RN 777063-42-0 CAPLUS
CN 1H-Pyrazole, 1-(3-methylbutyl)-4-(4-methylphenyl)- (CA INDEX NAME)

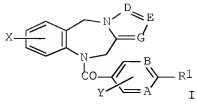


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

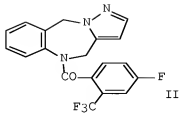
L16 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:71793 CAPLUS Full-text
DOCUMENT NUMBER: 138:122667
TITLE: Preparation of benzodiazepines as vasopressin agonists for the treatment of diabetes insipidus
INVENTOR(S): Dusza, John P.; Chan, Peter S.; Albright, Jay D.; Bagli, Jehan F.; Failli, Amedeo A.; Ashwell, Mark A.; Molinari, Albert J.; Caggiano, Thomas J.; Trybulski, Eugene J.
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S., 45 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6511974	B1	20030128	US 1998-122020	19980724
US 20030134845	A1	20030717	US 2002-320761	20021216
US 7138393	B2	20061121		
PRIORITY APPLN. INFO.:			US 1997-54252P	P 19970730
			US 1998-122020	A2 19980724

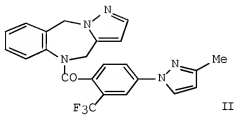
OTHER SOURCE(S): MARPAT 138:122667
GI



I



II



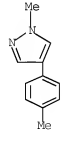
III

AB Title compds. I [A, B, E, G = CH, N; D = N, C-W; R1 = CN, CO2H, CONH2, etc.; X, Y = H, alkyl, cycloalkyl, etc.; W = H, halo, alkyl, etc.] and their pharmaceutically acceptable salts were prepd. For example, condensation of fluorobenzoyl II and the sodium salt of 3-methylpyrazol afforded claimed benzodiazepine III. In vasopressin V2 agonist studies of Brattleboro rats with central diabetes insipidus, 78-specific examples of compds. I exhibited urine vol. decrease ranging from 3-88%, e.g., benzodiazepine III decreased urine vol. by 80%. Compds. I are claimed useful for the treatment of diabetes insipidus, nocturnal enuresis, nocturia (sic), etc.

IT 37921-11-2P, 1-Methyl-4-(4-methylphenyl)-1H-pyrazole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of benzodiazepines as vasopressin V2 agonists for the treatment of diabetes insipidus)

RN 37921-11-2 CAPLUS

CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



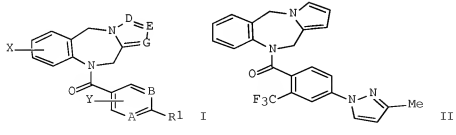
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:247184 CAPLUS Full-text
DOCUMENT NUMBER: 134:266333
TITLE: Preparation and formulation of aryl 5H,11H-pyrrolo[2,1-c][1,4]benzodiazepin-10-yl ketones and analogs as vasopressin agonists
INVENTOR(S): Yoon, Joseph Kyuwung; Saunders, Richard William; Fawzi, Mahdi Bakir
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: PCT Int. Appl., 154 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001022969	A2	20010405	WO 2000-US26380	20000926
WO 2001022969	A3	20011220		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6831079	B1	20041214	US 2000-669204	20000925
CA 2385971	A1	20010405	CA 2000-2385971	20000926
EP 1216045	A2	20020626	EP 2000-965432	20000926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003510280	T	20030318	JP 2001-526180	20000926
MX 2002003191	A	20020930	MX 2002-3191	20020326

PRIORITY APPLN. INFO.: US 1999-406165 A 19990927
US 1999-228814P P 19990927
WO 2000-US26380 W 20000926

OTHER SOURCE(S): MARPAT 134:266333
GI

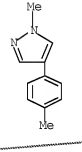


AB The title tricyclic vasopressin agonists (I) [wherein A, B, E, and G = independently CH or N; D = independently CW or N; R1 = alkanoyl, CN, CO2H, CONH2, C.tplbond.CH, C.tplbond.CR9, or (un)substituted 5-membered

heterocycles, such as pyrazolyl, imidazolyl, triazolyl, pyrrolyl, isoxazolyl, oxadiazolyl, or tetrazolyl; R9 = H, TMS, or alkyl; X and Y = independently H, (cyclo)alkyl perfluoroalkyl, alkoxy(alkyl), halo, or OH; W = H, halo, (alkoxy)alkyl, hydroxyalkyl, or CH2NR6R7; R6and R7 = independently H, alkyl, or taken together with the N to which they are attached form a pyrrolyl, piperidinyl, morpholinyl, alkylpiperazinyl, triazolyl, imidazolyl, or pyrazolyl ring; or a pharmaceutically acceptable salt thereof] were prepd. Thus, 4-fluoro-2-trifluoromethylbenzoyl chloride was coupled with 10,11-dihydro-5H-pyrrolo[2,1- c][1,4]benzodiazepine in CH2Cl2 to give (4-fluoro-2-trifluoromethylphenyl)(5H,11H-pyrrolo[2,1-c][1,4]benzodiazepin- 10-yl)methanone. 3-Methylpyrazole was treated with 60% NaH in DMF, the fluorophenyl deriv. added, and the mixt. heated in a sand bath at 110.degree.C for 15 h to afford II. Administration of 1-10 mg/kg of II to homozygous Brattleboro rats with central diabetes insipidus resulted in an 80% decrease in urine vol. and a 360% increase in urine osmolality. Thirty-two examples of formulations comprising from 1% to 20% of active ingredient, from 1% to 18% of a surfactant component, from 50% to 80% of a component of one or more polyethylene glycols, from 1% to 20% of a component of one or more sucrose fatty acid esters and/or polyvinylpyrrolidone and, optionally, one or more preservatives or antioxidants are also described. I are useful in the treatment of diabetes insipidus, nocturnal enuresis, nocturia, urinary incontinence, or bleeding and coagulation disorders, including hemophilia (no data).

IT 37921-11-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and formulation of aryl 5H,11H-pyrrolo[2,1-c][1,4]benzodiazepin-10-yl ketone vasopressin agonists by coupling aroyl halides with pyrrolobenzodiazepines)

RN 37921-11-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



102b, 103a

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:113685 CAPLUS Full-text
DOCUMENT NUMBER: 130:168402
TITLE: Preparation of N-benzoylpyrrolobenzodiazepines and analogs as vasopressin V2 receptor agonists
INVENTOR(S): Dusza, John Paul; Chan, Peter Sinchun; Albright, Jay Donald; Bagli, Jehan Framroz; Failli, Amedeo Arturo; Ashwell, Mark Anthony; Molinari, Albert John;

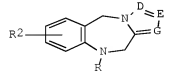
	Caggiano, Thomas Joseph; Trybulski, Eugene John
PATENT ASSIGNEE(S):	American Home Products Corporation, USA
SOURCE:	PCT Int. Appl., 133 pp.
	CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906409	A1	19990211	WO 1998-US15495	19980724
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2297406	A1	19990211	CA 1998-2297406	19980724
CA 2297406	C	20090224		
AU 9886633	A	19990222	AU 1998-86633	19980724
AU 756959	B2	20030130		
EP 1000062	A1	20000517	EP 1998-938017	19980724
EP 1000062	B1	20040922		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9811585	A	20000926	BR 1998-11585	19980724
HU 2000002480	A2	20001128	HU 2000-2480	19980724
HU 2000002480	A3	20020930		
JP 2001512125	T	20010821	JP 2000-505167	19980724
NZ 502449	A	20020828	NZ 1998-502449	19980724
RU 2213094	C2	20030927	RU 2000-104865	19980724
AT 277050	T	20041015	AT 1998-938017	19980724
CN 1183134	C	20050105	CN 1998-809641	19980724
ES 2229525	T3	20050416	ES 1998-938017	19980724
TW 502035	B	20020911	TW 1998-87112353	19980728
ZA 9806784	A	20000622	ZA 1998-6784	19980729
NO 2000000242	A	20000306	NO 2000-242	20000118
NO 315273	B1	20030811		
MX 2000000758	A	20010629	MX 2000-758	20000121

PRIORITY APPLN. INFO.:		US 1997-903369	A 19970730
		WO 1998-US15495	W 19980724

OTHER SOURCE(S): MARPAT 130:168402

GI



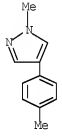
I

AB Title compds. [I; E,G = CH or N; D = (un)substituted CH or N; R = COZR1; R1 = cyano, CO2H, 1-alkynyl, azolyl, etc.; R2 = H, halo, alkyl, alkoxy, etc.; Z =

(un)substituted 1,4-phenylene, -pyridine- or -pyrimidine-5,2-diyl] were prepd. Thus, I (D-G = CH, R2 = H)(II; R = H) was amidated by 4-fluoro-2-trifluoromethylbenzoyl chloride and the product aminated by 3-methylpyrazole to give II [R = 4-(3-methyl-1-pyrazolyl)-2-trifluoromethylbenzoyl]. Data for biol. activity of I were given.

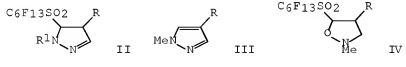
IT 37921-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of N-benzoylpyrrolobenzodiazepines and analogs as vasopressin V2 receptor agonists)

RN 37921-11-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:630403 CAPLUS Full-text
DOCUMENT NUMBER: 101:230403
ORIGINAL REFERENCE NO.: 101:34985a,34988a
TITLE: 1,3-Dipolar cycloadditions with .alpha.,.beta.-unsaturated fluoroalkyl sulfones
AUTHOR(S): Abad, E.; Fayn, J.; Bertaina, B.; Cambon, A.
CORPORATE SOURCE: Lab. Chim. Org. Fluor, Univ. Nice, Nice, F-06034, Fr.
SOURCE: Journal of Fluorine Chemistry (1984), 25(4), 453-64
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 101:230403
GI



AB The cycloaddn. of C6F13SO2CH:CHR (I; C6F13 = perfluorohexyl; R = C6H4OMe-4) with CH2N2 gave 74% of an 85-15 mixt. of pyrazolines II (R1 = H, Me). I (R = 2-furyl, 2-thiophenyl) and H2CN2 gave 80.5, 97.5% resp. of mixts. of II (R1 = Me) and pyrazoles III. Nitrone H2CN+(Me)O- underwent cycloaddn. with I (R =

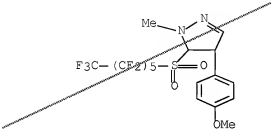
C6H4OMe-4, 2-furyl, 2-thiophenyl) to give 22-30% of the single products, isoxazolidines IV.

IT 93399-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 93399-98-5 CAPLUS

CN 1H-Pyrazole, 4,5-dihydro-4-(4-methoxyphenyl)-1-methyl-5-[(1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexyl)sulfonyl]- (CA INDEX NAME)



L16 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1984:85691 CAPLUS Full-text

DOCUMENT NUMBER: 100:85691

ORIGINAL REFERENCE NO.: 100:12997a,13000a

TITLE: 4-Phenylpyrazoles

PATENT ASSIGNEE(S): Grelan Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

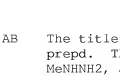
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58177977	A	19831018	JP 1982-57996	19820409

PRIORITY APPLN. INFO.: JP 1982-57996 19820409

GI



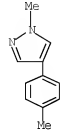
I

AB The title compds. I [R = alkyl, aryl; R1 = alkyl, HO2C, alkoxycarbonyl] were prepd. Thus, refluxing a mixt. of 12 g p-EtO2CC6H4C(:CHSMe)CHO, 4.416 g MeNHNH2, and 100 mL EtOH for 14 h gave 9.94 g I (R = Me, R1 = p-EtO2C).

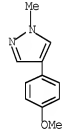
IT 37921-11-2P 82225-24-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

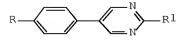
RN 37921-11-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



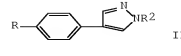
RN 82525-24-4 CAPLUS
CN 1H-Pyrazole, 4-(4-methoxyphenyl)-1-methyl- (CA INDEX NAME)



L16 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:562920 CAPLUS Full-text
DOCUMENT NUMBER: 97:162920
ORIGINAL REFERENCE NO.: 97:27177a,27180a
TITLE: A new and facile synthesis of 5-arylpyrimidines and 4-arylpyrazoles
AUTHOR(S): Kano, Shinzo; Yuasa, Yoko; Shibuya, Shiroshi; Hibino, Satoshi
CORPORATE SOURCE: Tokyo Coll. Pharm., Tokyo, 192-03, Japan
SOURCE: Heterocycles (1982), 19(6), 1079-82
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:162920
GI



I

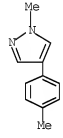


II

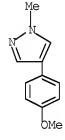
AB The cyclocondensation reaction of acroleins 4-RC6H4C(CHO):CHSMe (R = Me, OMe, F, Cl, CO2Et) with R1C(:NH)NH2 (R1 = H, Me, NH2) and R2NHNH2 (R2 = Me, Ph) gave the resp. pyrimidines I and pyrazoles II; I are useful as antiinflammatory agents (no data). Thus, a mixt. of 4-MeC6H4C(CHO):CHSMe, HC(:NH)NH2.cntdot.HOAc, and Na2CO3 in EtOH was refluxed to give I (R = Me, R1 = H).

IT 37921-11-2P 82525-24-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 37921-11-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



RN 82525-24-4 CAPLUS
CN 1H-Pyrazole, 4-(4-methoxyphenyl)-1-methyl- (CA INDEX NAME)



L16 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

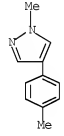
ACCESSION NUMBER:	1972:539882 CAPLUS Full-text
DOCUMENT NUMBER:	77:139882
ORIGINAL REFERENCE NO.:	77:23001a,23004a
TITLE:	Pyrazoles. IX. Nitration of 1-methyl-4-phenylpyrazole
AUTHOR(S):	Cohen-Fernandes, Pauline; Habraken, Clarisse L.
CORPORATE SOURCE:	Gorlaeus Lab., Univ. Leiden, Leiden, Neth.
SOURCE:	Recueil des Travaux Chimiques des Pays-Bas (1972), 91(9-10), 1185-92 CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB The phenyl and the pyrazole ring were both substituted on nitration with acetyl nitrate and a predominant ortho substitution in the phenyl ring was obsd. The pyrazole ring was susceptible to nitration at positions other than the, hitherto favored, 4-position.

IT 37921-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 37921-11-2 CAPLUS

CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



L16 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1960:110484 CAPLUS Full-text

DOCUMENT NUMBER: 54:110484

ORIGINAL REFERENCE NO.: 54:21054b-i,21055a-i,21056a-c

TITLE: The rearrangement of 3,3-disubstituted pyrazolenines

AUTHOR(S): Huttel, Rudolf; Franke, Karl; Martin, Hedwig; Riedl, Josef

CORPORATE SOURCE: Univ. Munich, Germany

SOURCE: Chemische Berichte (1960), 93, 1433-46
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 54:110484

AB cf. preceding abstr. The acid-catalyzed, alk., and thermal rearrangement of 3,3-disubstituted pyrazolenines to pyrazoles was, as far as the migration of the substituent to the C-4 atom was concerned, a sextet-rearrangement. This was concluded from a comparison of the rates of migration of various substituents. Me 3-methyl-3-phenylpyrazolenine-5-carboxylate (I) (100 mg.) heated slowly to 82-3.degree., and the resulting melt heated further to resolidify and then remelt at 143-6.degree. and recrystd. from petr. ether gave 60% Me ester (II) of 3-methyl-4-phenyl-5-carboxypyrazole (III), needles, m. 154.degree.. I boiled briefly in H2O gave 90% II, which kept 12 hrs. in cold glacial AcOH yielded 83% II, or refluxed 6 hrs. in MeOH gave 80% II. II (300 mg.) and 30 cc. 10% alc. NaOH kept overnight, dild. with H2O, neutralized with dil. HCl, and filtered, the filtrate evapd., the residue extd. with EtOH, and the residue from the ext. combined with the filter residue yielded 82% III, m. 253-4.degree. (decompn.) (EtOH), which decarboxylated gave at 255.degree./12 mm. 3-methyl-1-phenylpyrazole, m. 140-1.degree.. A small amt. of 3-phenyl-3-(p-bromophenyl) analog (IV) of I refluxed 0.5 hr. in MeOH and cooled gave a mixt. of Me ester (V) of 3-phenyl-4-(p-bromophenyl)pyrazole-5-carboxylic acid (VI) and Me 4-phenyl-3-(p-bromophenyl)pyrazole-5-carboxylate (VII). IV (4 g.) in 100 cc. EtOH refluxed 20 min., cooled, and fractionally concd. yielded 0.90 g. V, m. 229-32.degree., 1.78 g. mixt. of V and VII, and 0.43 g. yellowish residues. Fraction 2 sapond. and decarboxylated yielded a

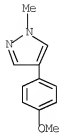
mixt. (m. 164.5.degree.) of 5.7% 3-phenyl-4-(p-bromophenyl)pyrazole (VIIa) (m. 155.degree.) and 94.3% 4-phenyl-3-(p-bromophenyl)pyrazole (VIII) (m. 166.3.degree.). V (0.9 g.) and 10 cc. 5% aq. alc. KOH refluxed while allowing the EtOH to evap., and the residual aq. soln. acidified with HCl gave 93% VI, m. 249-52.degree.. A small amt. of VI heated to 280.degree. until the gas evolution ceased, the resulting yellow glass boiled with ligroine, and the ext. concd. gave VIIa, needles, m. 133-4.degree.. Fraction 2 sapond. and decarboxylated gave a mixt., m. 141-61.degree., of VIIa and VIII. p-BrC6H4CH2COCl (70 g.) in 300 cc. dry C6H6 treated gradually with 40 g. AlCl3, refluxed 1 hr., cooled, poured onto 800 g. ice and 32 cc. concd. HCl, and filtered yielded 67% p-BrC6H4CH2COPh (IX), platelets, m. 146-7.degree. (MeOH). Dry HCO2Et (5 cc.) added with cooling to 1 g. Na in 15 cc. abs. EtOH, kept 3 hrs. in ice, treated with 12 g. IX, kept several days, dild. with 200 cc. iced H2O, filtered to remove 6.3 g. unchanged IX, acidified with dil. HCl, and filtered gave 68.5% p-BrC6H4CHBzCHO (X), m. 130-2.degree. (EtOH), violet with FeCl3. X (3.5 g.) in 100 cc. EtOH treated with stirring with 0.81 cc. 80% N2H4.H2O, heated briefly, concd., and refrigerated gave 2.55 g. VIIa, needles, m. 80-5.degree. resolidifying and remelting 151-3.degree., needles, m. 133-4.degree. (ligroine); the melt of the low-melting form seeded with the high melting form resolidified and rem. 155.degree.. p-BrC6H4COCH2Ph (XI) (12 g.) treated in the usual manner with HCO2Et gave 6.9 g. unchanged XI and 3.4 g. p-BrC6H4COCHPhCHO (XII), yellow needles, m. 107-8.degree. (EtOH), purple-red with FeCl3. XII (3 g.) treated in the usual manner with 0.8 cc. 80% N2H4.H2O yielded 57% VIII, needles which change shortly before melting to plates, m. 164-5.degree. (ligroine). 3-Methyl-3,5-diphenylpyrazolenine (XIII) (100 mg.) heated a few min. at 90.degree., cooled, and boiled with ligroine, and the ext. cooled yielded 85% 3-methyl-4,5-diphenylpyrazole (XIV), m. 175.degree. (EtOH or ligroine). XIII in glacial AcOH boiled briefly yielded 90% XIV; XIII kept in cold glacial AcOH gave 92% XIV; XIII treated with a few drops concd. H2SO4 yielded 55% XIV. The 5-(p-tolyl) homolog (XV) of XIII heated to 97.degree., boiled briefly in glacial AcOH, kept in cold glacial AcOH, or refluxed 6 hrs. in MeOH yielded 80, 90, 90, and 85%, resp., 5-(p-tolyl) homolog (XVI) of XIV, m. 170-1.degree. (EtOH or ligroine). PhCH2Ac (12 g.) and 8 g. NaNH2 in 200 cc. dry Et2O refluxed 4 hrs. with stirring while being treated with a stream of N, treated with stirring and cooling with 6 g. p-MeC6H4SO2Cl in Et2O, and acidified with dil. HCl, and the Et2O phase worked up gave 46% p-MeC6H4CHPhAc (XVII), m. 83-4.degree. (EtOH). XVII (1.5 g.) and 0.5 cc. 78% N2H4 in a few cc. EtOH heated 0.5 hr. on the water bath gave 74% XVI, needles, m. 171.degree. (EtOH or ligroine). Me 3,3,5-triphenylpyrazolenine-4-carboxylate (XVIII) (1 g.) in 10 vols. glacial AcOH heated 3 hrs. at 100.degree., poured into 40 cc. H2O, and filtered, and the residue crystd. from MeOH gave 33% Me 3,4,5-triphenylpyrazolecarboxylate (XIX), needles, m. 200-1.degree.; the mother liquor evapd. yielded 31% Me ester (XX) of 1,3,5-triphenyl-4-carboxypyrazole (XXI), m. 140-1.degree.. A similar run in glacial AcOH during 3 hrs. at 100.degree. gave 64% rearranged material consisting of 52% XIX and 48% XX; a run during 7.5 hrs. at 65.degree. gave 5.7% rearranged material consisting of 67% XIX and 33% XX. XVIII (1.18 g.) and the 5-fold amt. of maleic anhydride heated 10 hrs. at 100.degree. yielded 580 mg. XIX and 180 mg. XX. XVIII (500 mg.) treated with 1 cc. concd. H2SO4 and poured into H2O, and the ppt. fractionated from MeOH yielded 370 mg. 3,4,5-triphenylpyrazole (XXII), m. 265.degree., and 30 mg. XX. XVIII (500 mg.) heated 1 hr. at 190.degree. gave 340 mg. XX and 30 mg. XXII. XVIII heated 15 hrs. at 160.degree. yielded 84% product consisting of 14% XXII and 86% XX. XVIII heated 20 hrs. at 105.degree. gave 94% product consisting of 28% XIX and 72% XX. XVIII (500 mg.) refluxed 4 hrs. with 500 mg. KOH in 25 cc. MeOH, the mixt. dild. with H2O, and the ppt. recrystd. from MeOH gave 260 mg. XXII and 40 mg. unidentified material, C21H16O2, m. 127-8.degree.. XVIII and phthalic anhydride heated 4 hrs. at 135.degree. gave 83% product consisting of 40% XIX and 60% XX. XX (800 mg.) and 4.5 g. KOH in 35 cc. MeOH refluxed 2 hrs., poured into 250 cc. H2O, and acidified with dil. HCl gave 97% XXI, m. 238.degree.

(decompn.). XXI heated 0.5 hr. above the m.p. gave 79% XXII, m. 139-40.degree.. XIX refluxed 3 hrs. with KOH-MeOH and poured into H2O gave 86% XXII, m, 265.degree.. Me ester (XXIII) of 3-methyl-3,5-diphenylpyrazolenine-4-carboxylic acid (XXIV) in glacial AcOH heated 0.5 hr. on the water bath was recovered unchanged, but treated with a few drops cold concd. H2SO4 rearranged immediately to 3-methyl-4,5-diphenylpyrazole, m. 173-4.degree. (petr. ether), in 85% yield. XXIII (300 mg.) in alc. KOH kept at room temp. overnight, dild. with H2O, and neutralized with H2SO4 gave 58% XXIV, needles, m. 162-4.degree. (decompn.) (MeOH). XXIV (100 mg.) sublimed at 170.degree./12 mm. yielded 70% 3-methyl-4,5-diphenylpyrazole. 3-Methyl-3,5-diphenylpyrazolenine-4-carboxaldehyde (XXV) heated 1 hr. with glacial AcOH at 100.degree. was not rearranged. XXV heated briefly at 130.degree. resulted in partial rearrangement. XXV treated 1 min. at room temp. with concd. H2SO4 and dild. with H2O yielded 51% 3-methyl-4,5-diphenylpyrazole, m. 173.degree. (petr. ether). XXV treated 3 hrs. at 60.degree. with AgNO3 and NaOH yielded 60% XXIV, m. 163-4.degree. (decompn.). Di-Me 3-phenyl-3-(p-methoxyphenyl)pyrazolenine- 4,5-dicarboxylate (XXVI) (1 g.) and 10 cc. glacial AcOH refluxed 9 hrs. and poured into 50 cc. H2O, and the viscous ppt. fractionated from MeOH gave 550 mg. unchanged XXVI and 250 mg. Me ester (XXVII) of 3-phenyl-4-(p-methoxyphenyl)pyrazole-5-carboxylic acid (XXVIII), m. 238-9.degree.. A similar run in glacial AcOH during 27 hrs. at 100.degree. gave 9.5% XXVII. XXVI (712 mg.) heated 3.5 hrs. at 190.degree. and the residue fractionated from MeOH gave 403 mg. N-Me deriv. (XXIX) of XXVII, m. 114-15.degree., and 41 mg. XXVII. A similar run during 14 hrs. at 140.degree. gave 90% product consisting of 44% XXVII and 56% XXIX. A run during 27 hrs. at 120.degree. gave 36% XXVII. XXVI (500 mg.) treated with 2 cc. concd. H2SO4 and poured after 15 min. into 200 cc. H2O yielded 71.5% XXVII, m. 237.5-8.5.degree. (MeOH). XXVI (500 mg.), 600 mg. KOH, and 25 cc. MeOH refluxed 3 hrs., dild., and acidified gave 73% XXVIII, m. 219-20.degree. (decompn.), also obtained by sapon. of XXVII. XXVIII (400 mg.) heated 15 min. at 290.degree. yielded 76% 3-phenyl-4-(p-methoxyphenyl)pyrazole (XXX), cubes, m. 130-1.degree. (MeOH). XXIX (540 mg.) in 30 cc. MeOH refluxed 0.5 hr. with 400 mg. KOH, poured into 100 cc. H2O, filtered, and acidified gave 81% N-Me deriv. (XXXI) of XXVIII, needles, m. 132.5-3.5.degree.. XXXI (340 mg.) heated 0.5 hr. at 250-60.degree. gave 210 mg. N-Me deriv. (XXXIa) of XXX, cubes, m. 132.5-3.5.degree. (MeOH). Dry HCO2Et (1.7 g.) added with cooling to 0.5 g. Na in 18 cc. abs. EtOH, kept 3 hrs. at 0.degree., treated with 3 g. p-MeOC6H4CH2Bz, kept overnight at 0.degree. with occasional shaking and then 3 days at room temp., poured into 100 cc. iced H2O, filtered and acidified with cold, dil. H2SO4 pptd. 2.6 g. p-MeOC3H4CHBzCHO (XXXII), m. 114-15.degree. (MeOH), violet-brown with FeCl3. XXXII (2.6 g.) in EtOH refluxed 45 min. with 0.6 cc. 78% N2H4.H2O, dild. with H2O, and extd. with Et2O, and the ext. evapd. yielded 2 g. XXX, m. 131-2.degree. (ligroine). XXX (750 mg.), 20 cc. N NaOH, and 1 g. Me2SO4 shaken 4 hrs. with cooling, and heated to 60-70.degree., and the crude product recrystd. from MeOH yielded 540 mg. XXXIa, cubes, m. 132-3.degree.. HCO2Et (2.5 cc.), 0.5 g. Na, and 20 cc. abs. EtOH treated in the usual manner with 4.5 g. p-MeOC6H4COCH2Ph yielded 4.2 g. p-MeOC6H4COCHPhCHO (XXXIII), m. 81-2.degree.. XXXIII (2.5 g.) treated in the usual manner with N2H4.H2O yielded 58% 4-phenyl-3-(p-methoxyphenyl)pyrazole, needles, m. 127-7.5.degree. (ligroine).

IT 113014-09-8P, Pyrazole, 4-(p-methoxyphenyl)-1-methyl-3(or 5)-phenyl-
RL: PREP (Preparation)
(prepn. of)

RN 113014-09-8 CAPLUS

CN Pyrazole, 4-(p-methoxyphenyl)-1-methyl-3(or 5)-phenyl- (6CI) (CA INDEX NAME)



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Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	85.10	467.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-12.30	-22.14

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 11:19:07 ON 24 APR 2009